1H-Indene, 2-methyl-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 102

Global applicability domain: Inside

Local applicability domain index: 6.20e-01

Confidence level: 6.74e-01

Nearest Neighbors from the Training Set

Image not found

2,5-Dimethyl-2,4-hexadiene
Measured: 209
Predicted: 175

Image not found

4-Vinylcyclohexene
Measured: 166
Predicted: 158

Image not found

5-Ethylidene-2-norbornene
Measured: 110
Predicted: 134

Image not found

2,4,4-Trimethyl-1-pentene
Measured: 603
Predicted: 347

Image not found

Isophorone
Measured: 2.00
Predicted: 3.19